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# Performance of electrochemical cell with various flow channels for Bunsen reaction in the sulfur–iodine hydrogen production process



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## ARTICLE INFO

## ABSTRACT

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Renewable hydrogen production through sulfur–iodine (SI) cycle is energy efficient and environmentally friendly. Electrochemical cell (EC) has recently been proposed to carry out the Bunsen reaction in the cycle. Existing studies on the EC are limited only to time-consuming experiments whereas cell performance with respect to flow channel is very few. In this study, numerical study is conducted for determining the impact of flow channel on the EC performance of electrochemical Bunsen reaction. Five different configurations of flow channel are physically modelled. A three dimensional, steady state and laminar flow through EC is simulated by solving the governing equations, and show good agreement with experimental data at low current density. It is found that the flow field, local current and potential of serpentine, straight parallel and spiral tubular flow channels distribute almost uniformly, except the significant vortex regions and high resistance at the square bends of straight parallel channel due to the sudden geometric changes. The flow maldistribution in Z-type and U-type parallel flow channels makes them unsuitable for EC. The straight parallel flow channel is found to be optimal due to its low pressure drop as well as low electric power input, followed by serpentine and spiral tubular patterns. The simulation concerning flow channels design favors improving EC performance and the thermal efficiency of SI cycle.

### 1. Introduction

Large consumption of fossil fuels and accompanying environmental pollution are influencing the economic and social development in the world. Hydrogen as a clean, highly-effective, sustainable energy carrier is considered to be a promising alternative [\[1\].](#page--1-0) It can meet the worldwide energy demand and meanwhile reduce  $CO<sub>2</sub>$  and pollutants emissions. There is a rapid growth in hydrogen utilization as transportation, power generation and fuel cell [\[2\].](#page--1-1) Several ways for mass production of hydrogen are coal gasification, natural gas reforming and water electrolysis. Nevertheless, there is a growing development on renewable hydrogen production technologies [\[3\].](#page--1-2) Among these, the sulfur–iodine (SI) thermochemical water-splitting cycle assembled with nuclear or solar energy has been explored as a promising process for large-scale and high-efficient hydrogen production [\[4,5\]](#page--1-3).

<span id="page-0-1"></span>The schematic diagram of the SI cycle is presented in [Fig. 1,](#page-1-0) mainly consisting of the following three reactions [\[6\]:](#page--1-4)

$$
SO_2 + I_2 + 2H_2 O \xrightarrow{293-393 \text{ K}} H_2SO_4 + 2H I
$$
 (1)

$$
H_2SO_4 \xrightarrow{1073-1273 \text{ K}} SO_2 + H_2 O + 0.5O_2 \tag{2}
$$

$$
2\text{H1} \xrightarrow{573-773 \text{ K}} \text{H}_2 + \text{I}_2 \tag{3}
$$

The net reaction for Bunsen reaction  $(1)$ , H<sub>2</sub>SO<sub>4</sub> decomposition  $(2)$ and HI decomposition (3) is the splitting of water to hydrogen and oxygen, while the intermedium of  $SO_2$  and  $I_2$  recycle in the SI cycle. Due to the positive Gibbs free energy change ( $\Delta G_{400\mathrm{K}}^{0}$ ) of  $+82$  kJ/mol in the stoichiometric Bunsen reaction, excessive water is always employed for diluting the products and making  $\Delta G_{400\mathrm{K}}^{0}$  negative [\[7\].](#page--1-5) Thus the reaction becomes thermodynamically favorable. To separate the produced H2SO4 and HI, GA first proposed a traditional method of using excessive iodine [\[6\]](#page--1-4). The complexation between iodine and iodide leads to the spontaneous separation of  $H_2SO_4/HI/I_2/H_2O$  quaternary mixture into two phases:  $H_2SO_4/H_2O$  in the upper sulfuric acid phase,  $H_1/I_2$ /  $H<sub>2</sub>O$  in the lower poly-hydroiodic acid phase [\[8\]](#page--1-6). However, the large excess amounts of iodine and water dilute the acids and meanwhile unexpected impurities always exist in two phases, which require further separation, purification, concentration and recycling before the decomposition of  $H_2SO_4$  and HI [9–[11\]](#page--1-7). As a result, the flowsheet of traditional SI cycle is complicated and energy-extensive, putting off the industrialization of SI cycle.

Alternative routes for carrying out Bunsen reaction have been

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<span id="page-1-0"></span>

Fig. 1. Schematic diagram of the sulfur–iodine cycle for hydrogen production.

proposed in recent years, including electrochemical, reaction in nonaqueous solvents and chemical precipitation [12–[14\]](#page--1-8), to overcome the disadvantages of traditional Bunsen reaction. Application of an electrochemical cell (EC) to Bunsen reaction was put forward by Nomura et al. [\[12\].](#page--1-8) A proton exchange membrane separates the anode and cathode in the EC and meanwhile allows the transport of proton from anode to cathode. The electrode reactions are presented in Eqs. [\(4\) and](#page-1-1)  $(5)$ , where SO<sub>2</sub> is oxidized at anode and I<sub>2</sub> is reduced at cathode with the supply of electric power. The concentrated  $H_2SO_4$  and HI solutions with less impurities generate separately in the EC [\[15\],](#page--1-9) decreasing the required excess amounts of  $I_2$  and  $H_2O$  significantly. Moreover, the liquid-liquid equilibrium (LLE) phase separation and the mass recycling of excessive substance employed in the traditional Bunsen reaction can be eliminated. Once the impurities in the  $H_2SO_4$  and HI solutions of EC are minimized and negligible through optimizing membrane type and cell configuration, the extra purification of solutions will be cancelled. Especially if an over-azeotropic  $HI/H<sub>2</sub>O$  solution is obtained [\[16\]](#page--1-10), the energy-intensive processes of EED or extractive distillation for concentrating HI can be omitted as well, which will significantly reduce the energy consumption of SI cycle.

<span id="page-1-1"></span>Anode: 
$$
SO_2 + 2H_2 O \rightarrow H_2 SO_4 + 2H^+ + 2e^-
$$
 (4)

Cathode: 
$$
I_2 + 2H^+ + 2e^- \rightarrow 2HI
$$
 (5)

Experimental work on the electrochemical Bunsen reaction has focused on its fundamental characteristics [\[12,15](#page--1-8)–22], including acid concentration, membrane transport properties, electric energy consumption, kinetics, etc. 93% of excess iodine and 69% of excess water with respect to the traditional Bunsen reaction can be reduced using this technique [\[12\].](#page--1-8) The thermal efficiency of the new SI cycle assembled with electrochemical method has been preliminarily estimated to be 42.1% and can be further improved [\[16\].](#page--1-10) To-date, parametric studies on the influence of flow channel on the cell performance of EC have not been carried out. The flow channel of electrolyte at anode and cathode should be optimized to obtain a uniform distribution of flow, the optimal minimal pressure drop and electric power input. However, the cost and time consumed in manufacturing EC with various flow channels for experimental studies are quite high. Hence, numerical study gives an opportunity to optimize qualitatively the design of flow channels.

Researches on the gas flow channel design of fuel cell, where chemical energy is directly converted to electrical energy, have been reported widely. In the review paper of Manso et al. [\[23\],](#page--1-11) a detailed explanation on the effects of geometric flow channels on the performance enhancement of proton exchange membrane fuel cell (PEMFC) has been proposed. Saco et al. [\[24\]](#page--1-12) carried out numerical study for

optimizing the flow channels with respect to optimal pressure drop and water management of PEMFC. These studies on the fuel cell suggest the significance of flow channel design.

Up to now, there is no mathematical modeling study on electrochemical Bunsen reaction found in the literature. This work investigates numerically the performance of EC with five different configurations of flow channel, involving serpentine, straight parallel, Z-type parallel, Utype parallel and spiral tubular. The flow and electrochemistry coupling characteristics in the EC are evaluated, especially the distribution of flow field, electric field, pressure drop across flow channel and electric power consumption, to optimize the flow channel design and operation of electrochemical Bunsen reaction.

#### 2. Theoretical

#### 2.1. Physical model

The simplified electrochemical cell (EC) for carrying out Bunsen reaction is shown in [Fig. 2,](#page-1-2) mainly including anode, cathode, flow channel, anolyte and catholyte, and a proton exchange membrane (Nafion 117). The electric power to the EC is supported by a D.C. supply. Five different configurations of flow channel namely (a) serpentine (b) straight parallel (c) Z-type parallel (d) U-type parallel and (e) spiral tubular are modelled, as shown in [Fig. 3](#page--1-13). The inlet and outlet

<span id="page-1-2"></span>

Fig. 2. Schematic diagram of the electrochemical cell.

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